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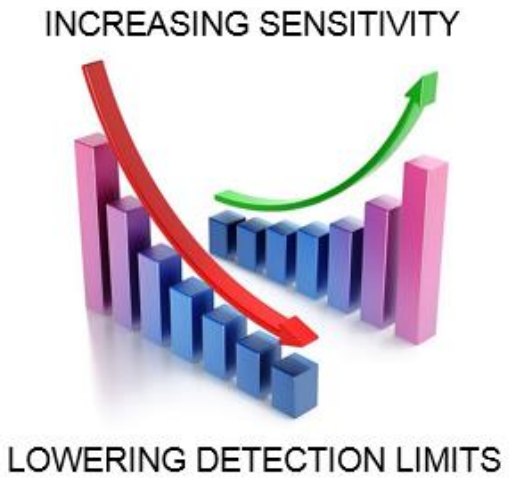
Single, Triple or High Resolution Accurate Mass? Select the Right GC-MS for Your Lab

Factors to Consider

- Number of samples & analytes to be monitored
- Sample variability (matrix)
- Need for high capacity methods
- Regulations
- Sensitivity, Selectivity, Budget, Ease of Use, Flexibility
- High-throughput capability
- Reduced cost/analysis
- Known vs unknown identification



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Thermo Scientific GC/GC-MS Portfolio

Thermo Scientific™ TRACE™ 1300 Series GC Systems	Thermo Scientific™ ISQ™ Series GC-MS Systems	Thermo Scientific™ TSQ™ Series GC-MS & MS/MS Systems	Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS System	Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS System
Laboratory GC Multiple detectors and inlets	Single Quadrupole MS	Triple Quadrupole MS	Hybrid Quadrupole – Orbitrap GC-MS & GC-MS/MS	Double focusing Magnetic sector
Detection with Multiple Detectors	Confirmation by Mass Spectrum or SIM	High speed and high capacity MS/MS and SRM	High Resolution and Accurate Mass Full scan and MS/MS	High resolution selected ion recording (SIR)
General organics, pollutants, purity assays,	EPA Regulated Methods (524, 525, 8260, 8270)	Target Analysis requiring ultimate sensitivity/selectivity	Simultaneous quantitative and qualitative analysis with high selectivity	High Resolution targeted quantitation and general analytical work
QA/QC, Petro, Toxicology, Environmental	Environmental, general organic, forensic chemistry and toxicology	Food Testing, Environmental, Antidoping, steroids analysis	Food safety, environmental, 'omics, industrial, forensic tox , doping, pharma	Persistent organic pollutants (POPs) , sports doping, petrochem

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Using Mass Spectrometers as Detectors in GC – Single Quadrupoles

GC-MS Single Quadrupoles

GC-MS: An analyte is identified and quantified by the area or height of a peak from the signal of an ion with a specific m/z ratio at an expected retention time.

- Produces reproducible mass spectra of all compounds with fragmentation fingerprint
- Combine with retention time for positive identification
- Accurate and reproducible results at the low levels
- Full scan for library searching
- Alternating full scan/SIM for unknowns and low level analysis
- Capable of both EI and CI ionization
- DIP and DEP Probe Analysis
- Easy to Use and Maintain
- High sensitivity in SIM
- Reference Libraries

Thermo Scientific™ ISQ™ 7000 GC–MS system

ThermoFisher SCIENTIFIC

Familiar Territory

- Single Quadrupole GC-MS
- Staple of the analytical laboratory
- Hugely diverse range of applications
- Sensitive
- Rugged
- Routine workhorse

Thermo Scientific™ ISQ™ 7000 GC–MS system

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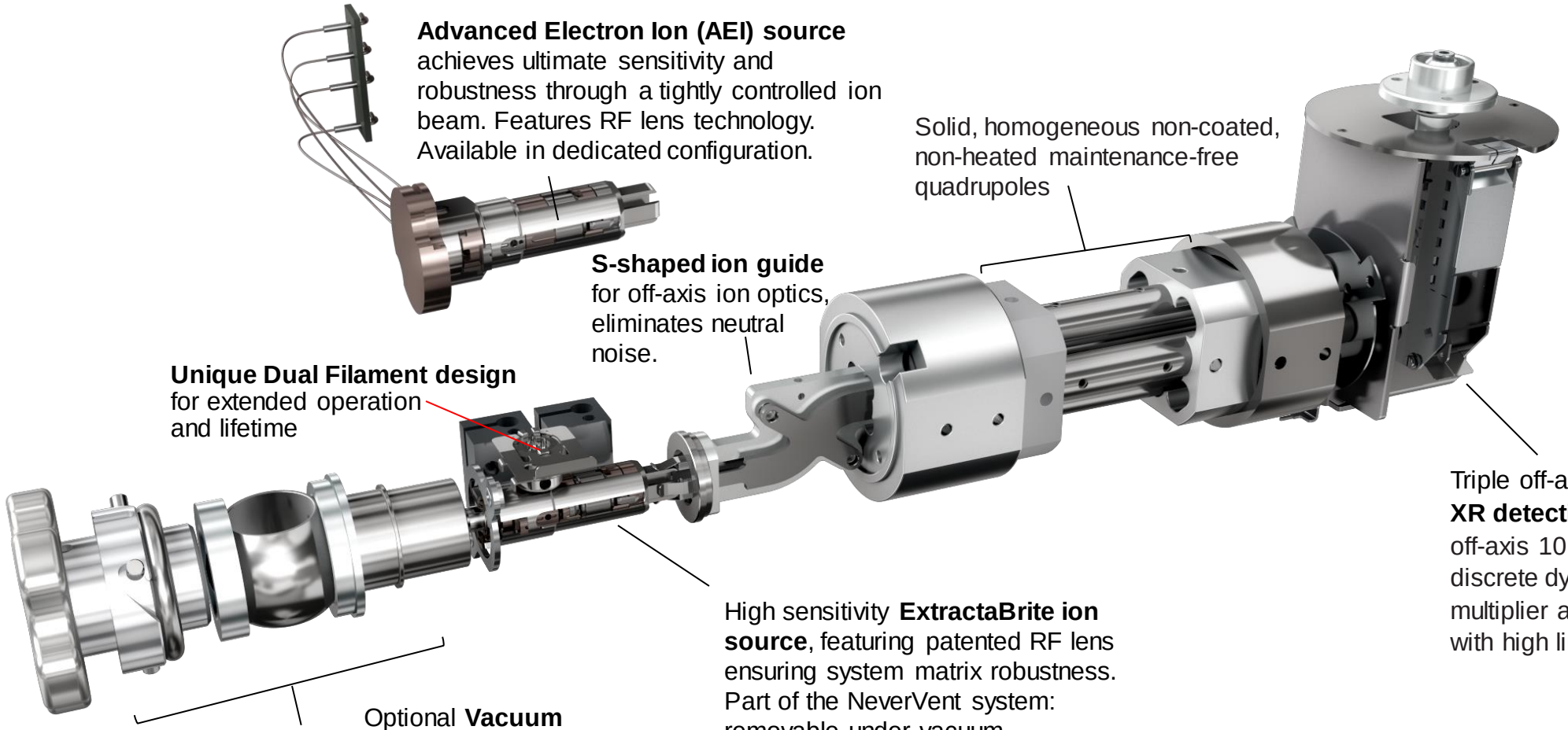
Anatomy of a Single Quad



Advanced Electron Ion (AEI) source achieves ultimate sensitivity and robustness through a tightly controlled ion beam. Features RF lens technology. Available in dedicated configuration.

Solid, homogeneous non-coated, non-heated maintenance-free quadrupoles

S-shaped ion guide for off-axis ion optics, eliminates neutral noise.

Unique Dual Filament design for extended operation and lifetime

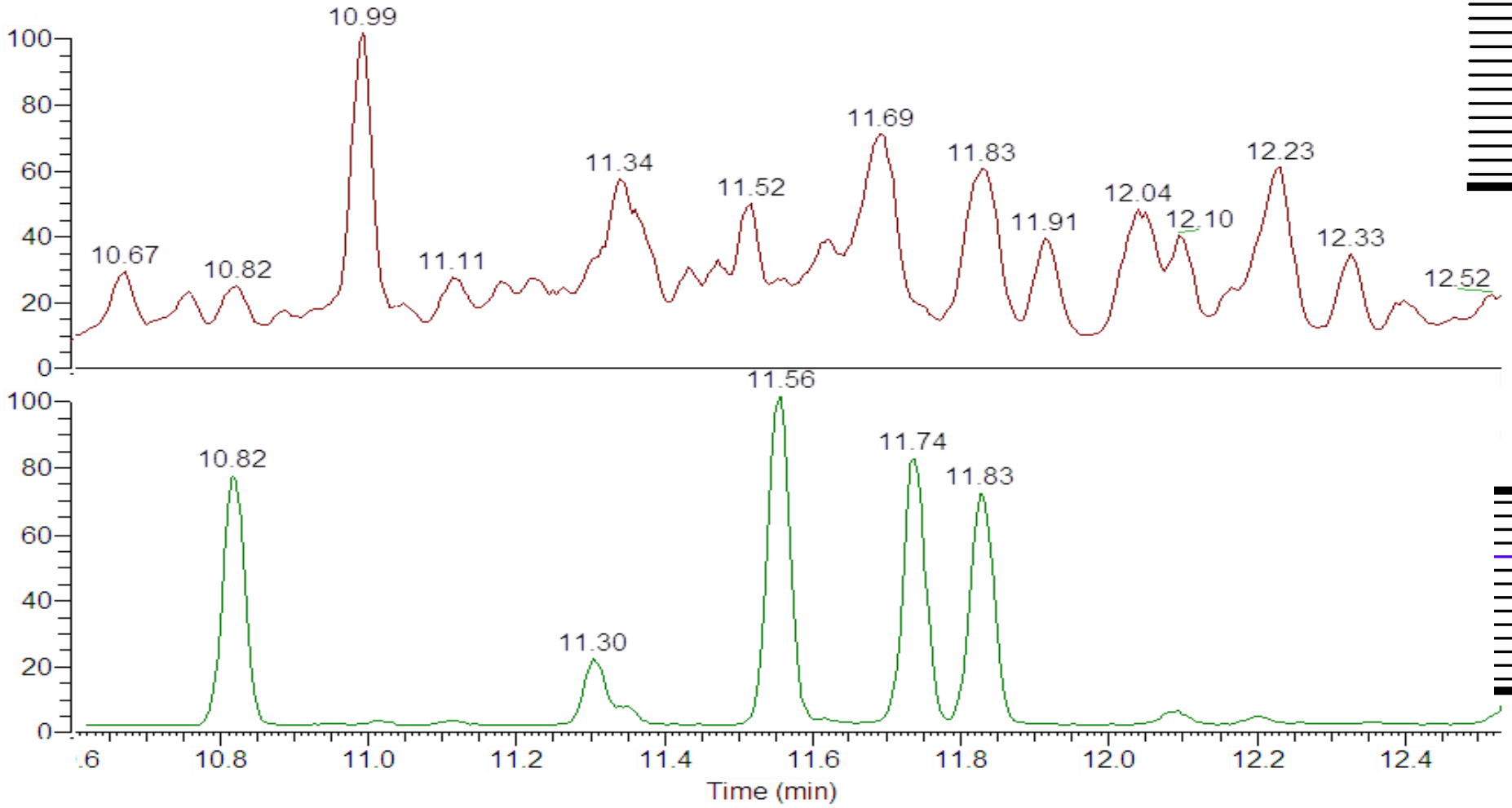
Triple off-axis **DynaMax XR detection system**, with off-axis 10 kV dynode, discrete dynode electron multiplier and electrometer with high linear range

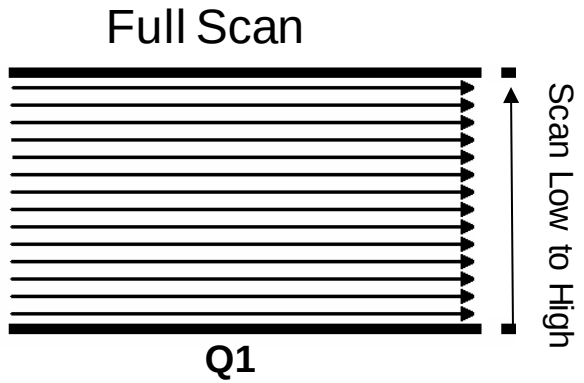
High sensitivity **ExtractaBrite ion source**, featuring patented RF lens ensuring system matrix robustness. Part of the NeverVent system: removable under vacuum

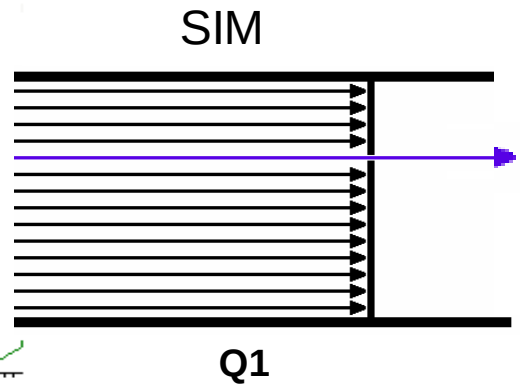
Optional **Vacuum Probe Interlock (VPI)** enables NeverVent technology

Single Quad GC-MS: Two Common Acquisitions

Full Scan: Shows all of the ions that are being formed in the ion source

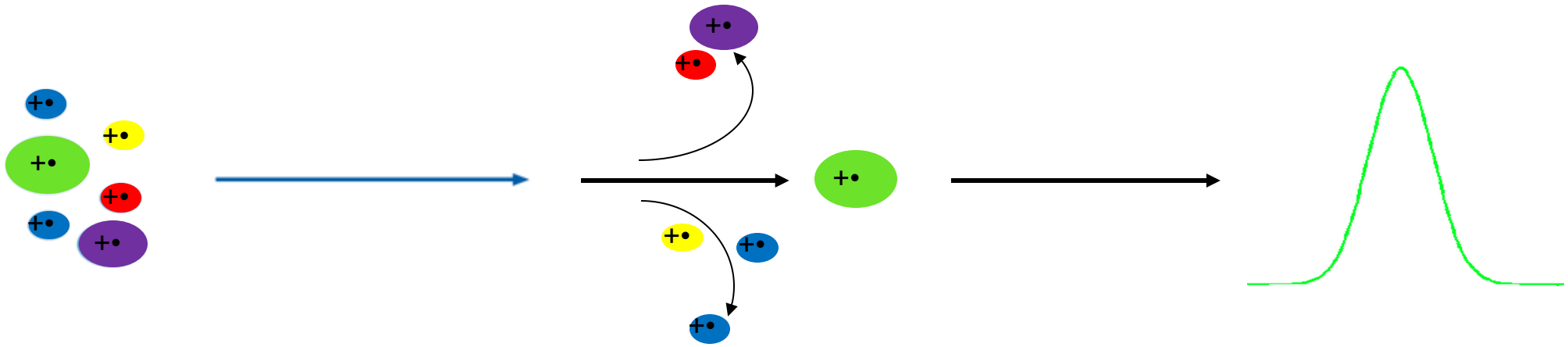


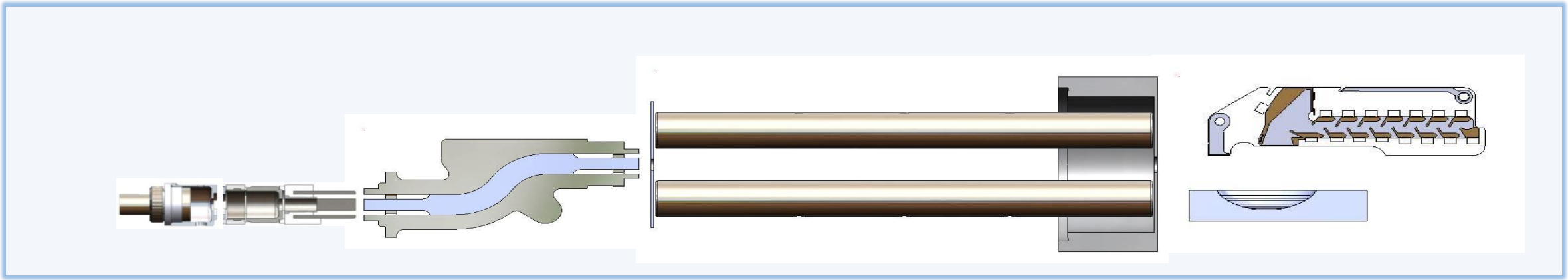




SIM: Provides the best sensitivity for quantitation plus increased selectivity

Single Quad GC-MS: Mass (*m/z*) Filtration SIM (Selected Ion Monitoring)

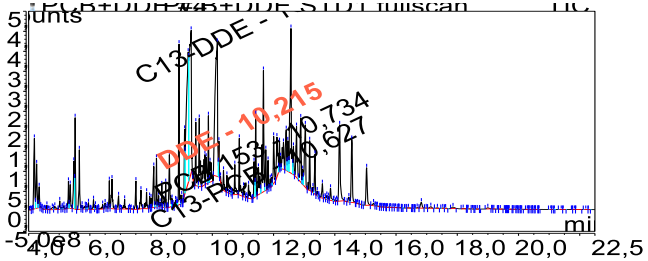




SIM - acquisition mode, commonly used on single quadrupole systems, where a single mass (m/z) or series of masses is specified by the user for targeting.

But What if I Still Have a Coeluting Matrix Peak with the Same m/z Ratio?

- If better separation, selection of m/z ion or ionization technique doesn't help? Then we need to add mass spectrometry tools to increase selectivity to be able to find our compound of interest.



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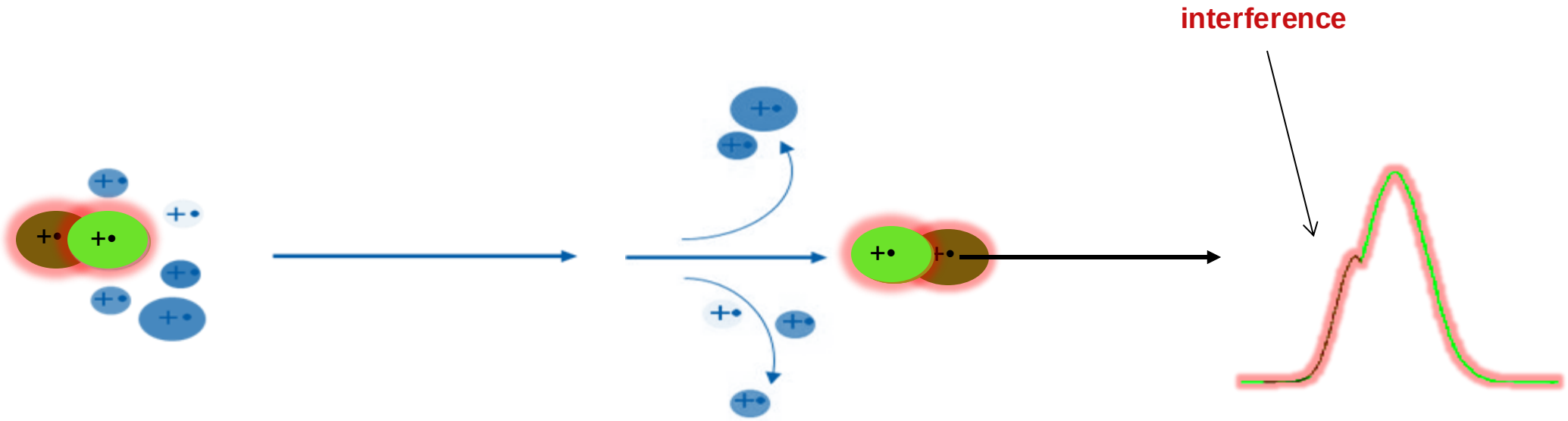
Single Quadrupole “Real Life” SIM in Complex Matrix



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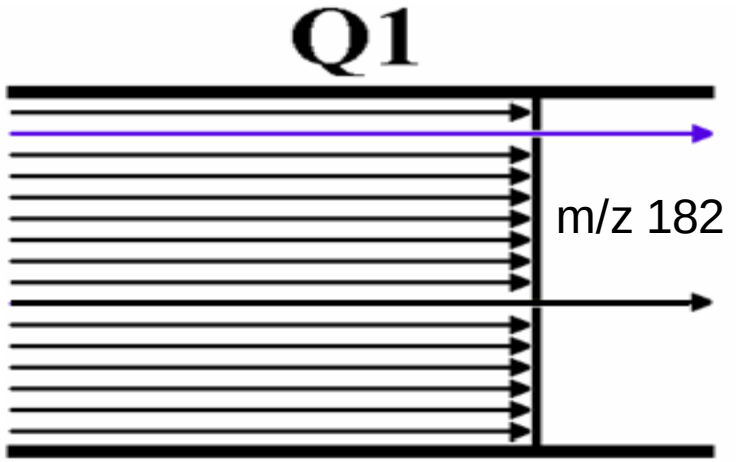
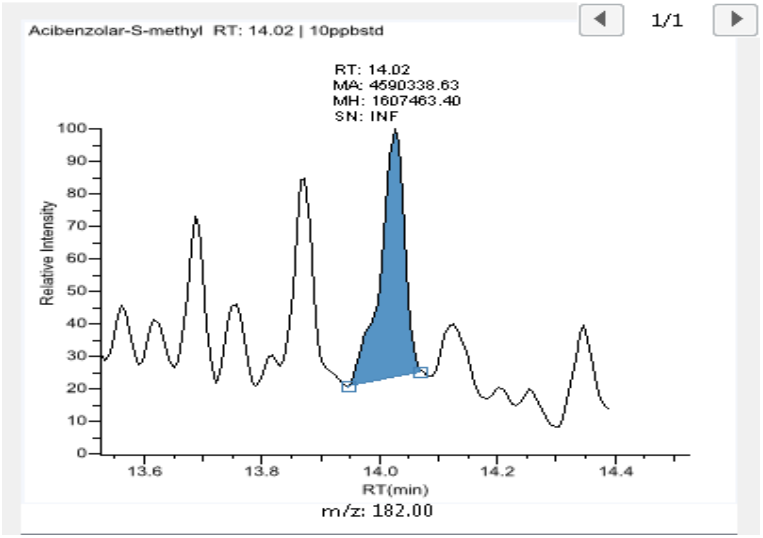
Reaching the Boundaries of What Single Quadrupoles Can Offer



Selected analyte precursor ion

Matrix ion with same mass number



SIM on m/z 182

- Leads to systematic errors
  - Biases
- Can cause false positive results
- Can raise LODs
- Reduce signal/noise

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Using Mass Spectrometers as Detectors in GC – Triple Quadrupoles

GC-MS/MS: Triple Quadrupoles

GC-MS/MS: Another dimension is added by choosing a specific ion from the EI or CI spectra and allow that "precursor ion" to fragment using an optimized energy. The "product ion" formed this way is then used for quantitation. This process is known as **Selective Reaction Monitoring** (SRM)

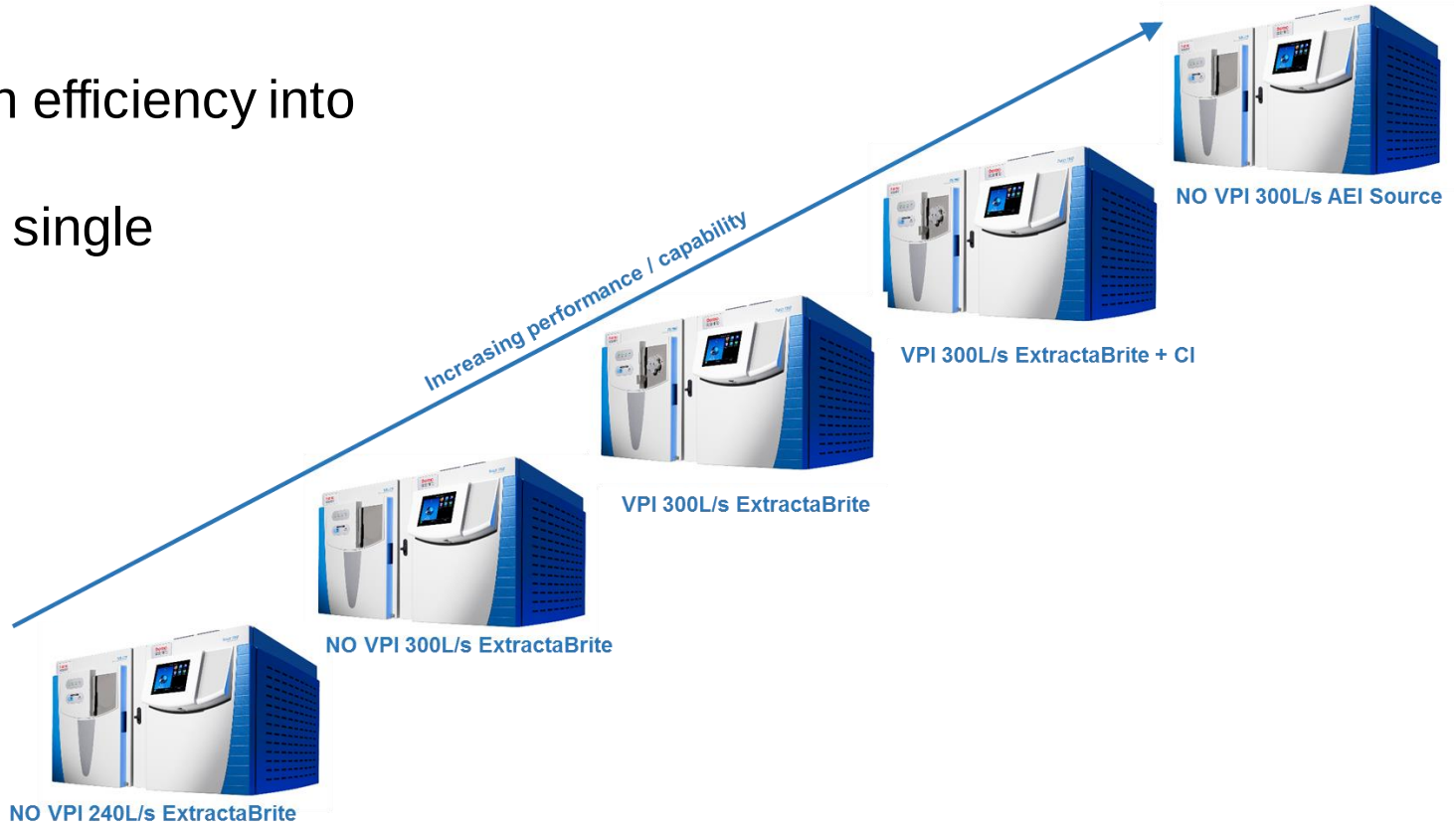
- Low level analysis in heavy matrix for 100's of compounds in SRM
- Excellent for High capacity methods
- Targeted analysis and screening
- Dramatic reduction of signal from the matrix (increased S/N)
- Great precision at low concentration in matrix
- Can be used in Single Quad Mode
- Full scan for library searches
- Alternating full scan/SRM for unknowns and low level analysis
- Capable of EI and CI Ionizations
- DIP and DEP Probe Analysis
- More Selectivity when compared to SQ

Thermo Scientific™ TSQ™ 9000 GC –MS /MS system

ThermoFisher SCIENTIFIC

Completely Scalable Future Proof Investment

- Excellent Performance
  - Selected Ion Monitoring (SIM)
  - Full Scan
  - Selected Reaction Monitoring (SRM)
  - Other MS/MS modes
- GC- Triple Quad selectivity can bring high efficiency into lab workflows
- SQ > TQ method migration possible on a single platform
- Advantages
  - Continue current methods
  - Switch at the right time in a “safe” way
  - Future-proof approach



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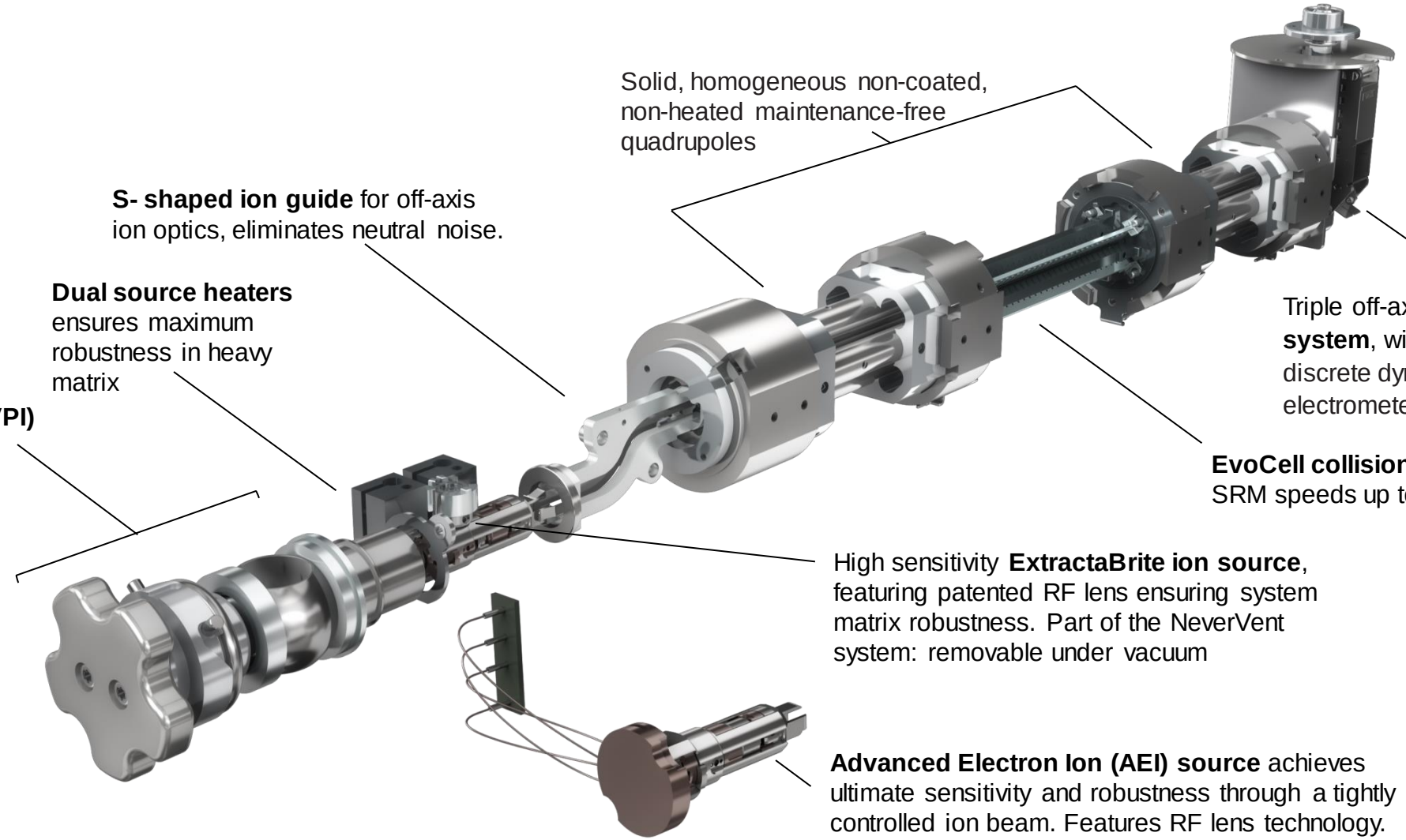
Anatomy of a Triple Quad



Solid, homogeneous non-coated, non-heated maintenance-free quadrupoles

S- shaped ion guide for off-axis ion optics, eliminates neutral noise.

Dual source heaters ensures maximum robustness in heavy matrix

Optional **Vacuum Probe Interlock (VPI)** enables NeverVent technology

Triple off-axis **DynaMax XR detection system**, with off-axis 10 kV dynode, discrete dynode electron multiplier and electrometer with high linear range

EvoCell collision cell for high SRM speeds up to 800 SRM/s

High sensitivity **ExtractaBrite ion source**, featuring patented RF lens ensuring system matrix robustness. Part of the NeverVent system: removable under vacuum

Advanced Electron Ion (AEI) source achieves ultimate sensitivity and robustness through a tightly controlled ion beam. Features RF lens technology. Available in dedicated configuration.

How Does Triple Quadrupole GC-MS/MS Differ from Single Quadrupole GC-MS?

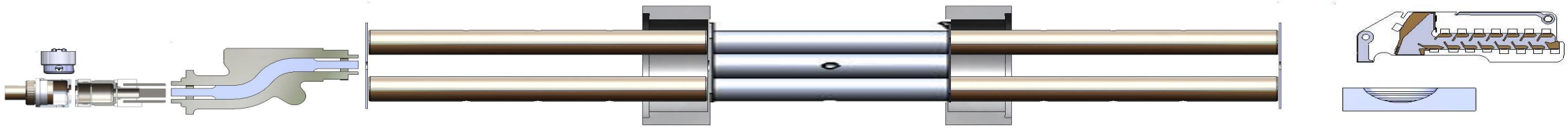
Single Quadrupole GC-MS

MS

Ion Source | **Ion Transfer Optics** | **Quadrupole** | **EM Detector**

Triple Quadrupole GC-MS/MS

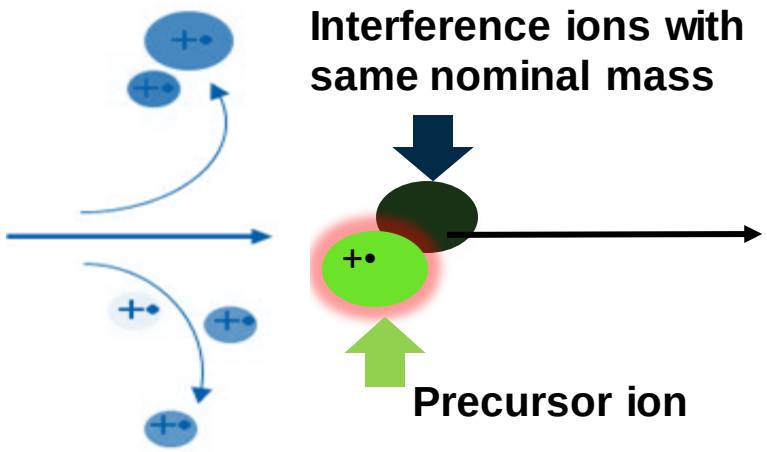
MS **MS**

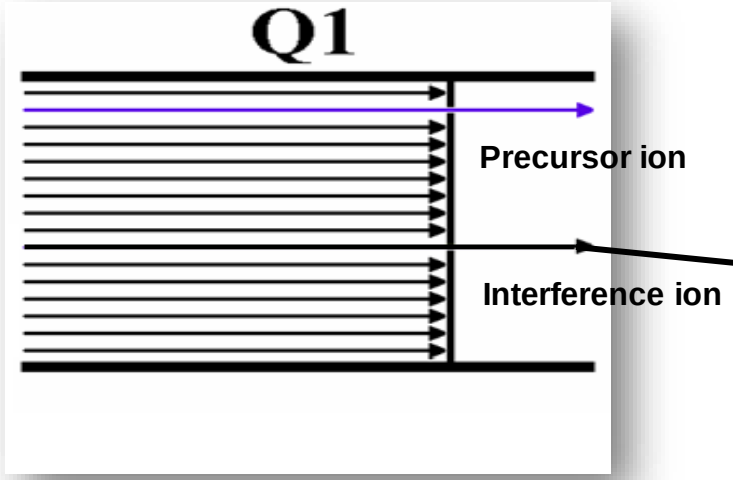


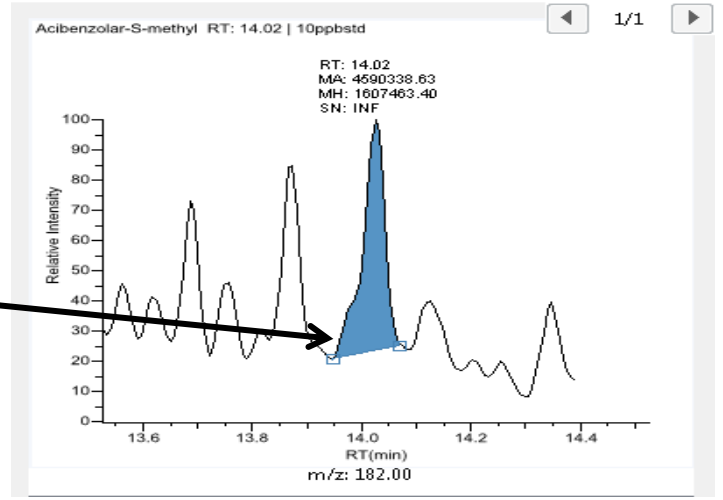
Ion Source | **Ion Transfer Optics** | **Quadrupole 1 (Q1)** | **Quadrupole 2 (Q2) Collision Cell** | **Quadrupole 3 (Q3)** | **EM Detector**

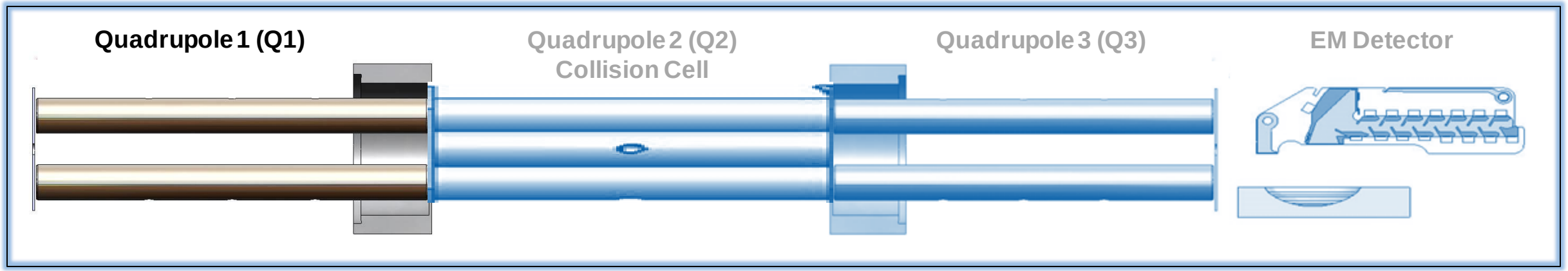
Triple Quad GC-MS: Q1 Precursor Ion Selection

Significant contribution from matrix ion causes peak area to be too high









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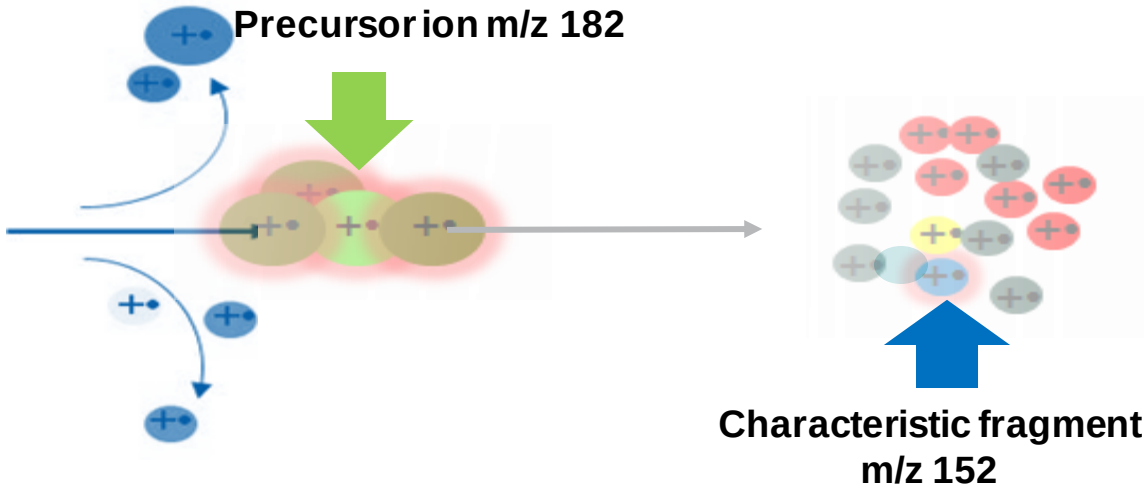
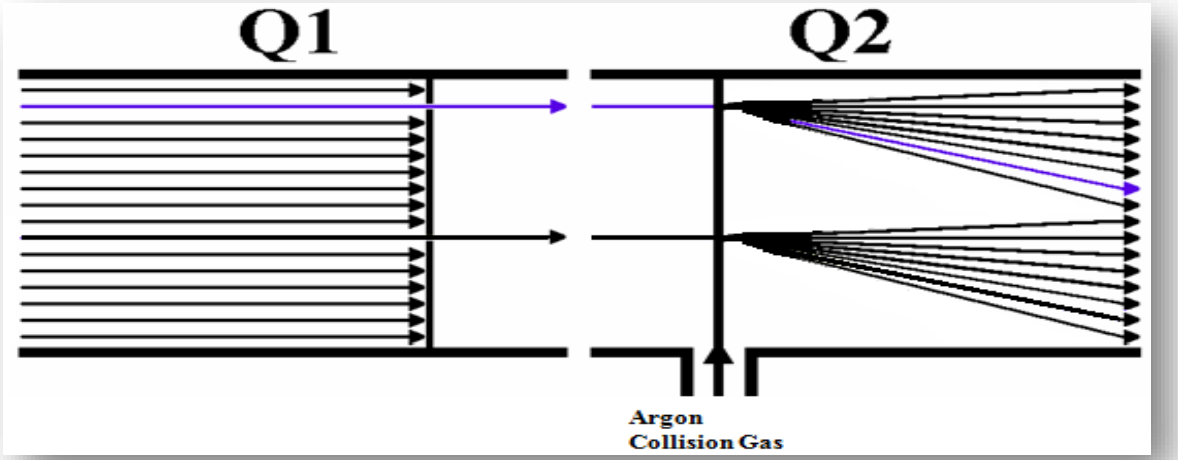
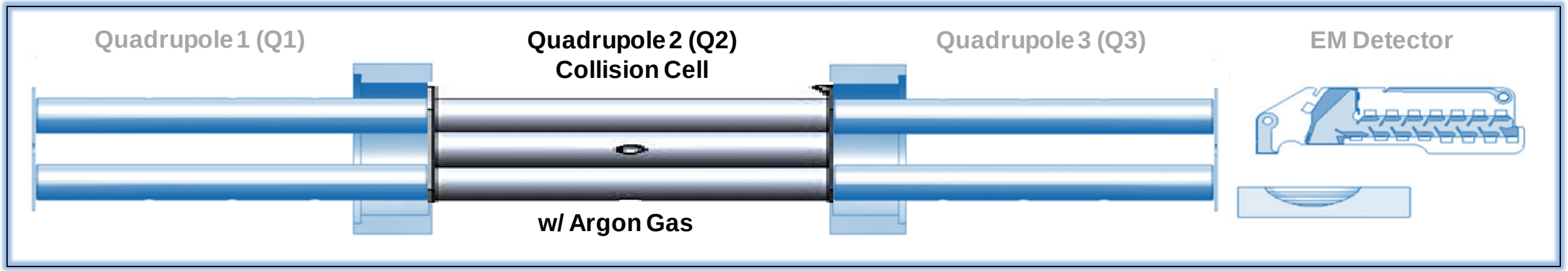
Triple Quad: Q2 Collision-Induced Dissociation (CID)

Fragmentation of both analyte and matrix ion







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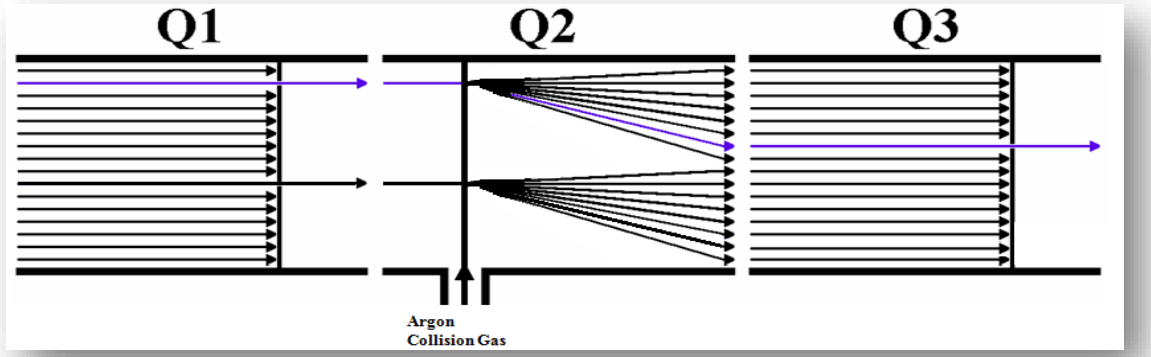
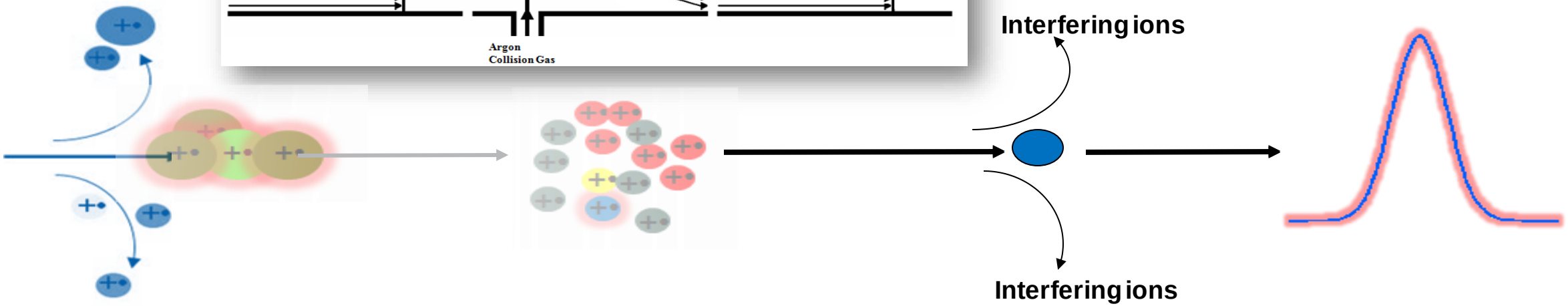
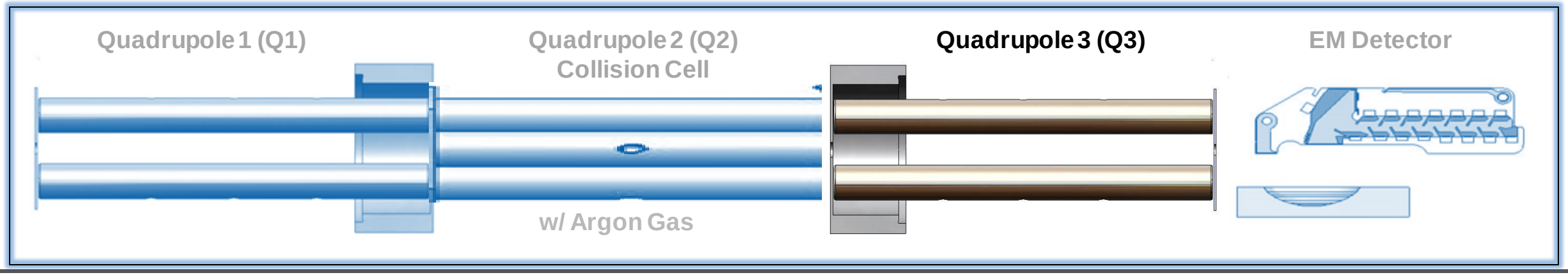
Triple Quad GC-MS: Q3 Product Ion Selection



Selection of unique product ion of analyte





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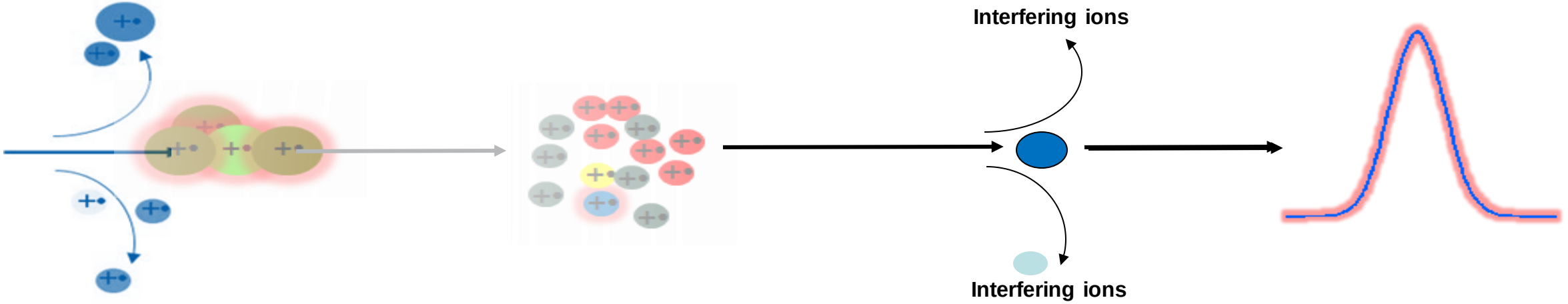
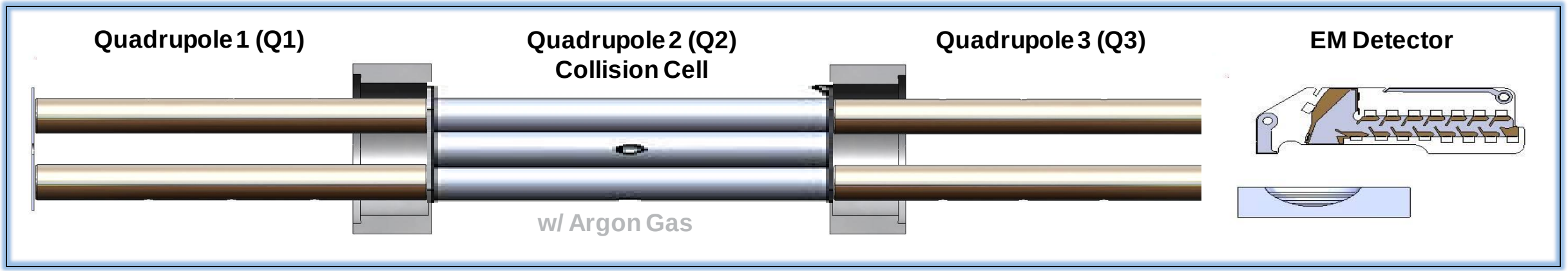
Triple Quad GC-MS: Selected Reaction Monitoring (SRM)





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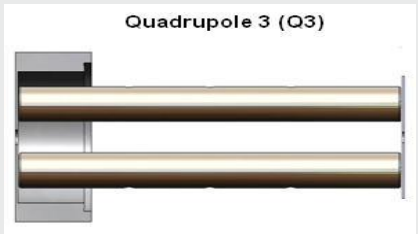
SRM Goal…Find the Most Selective, Intense Transition/Compound

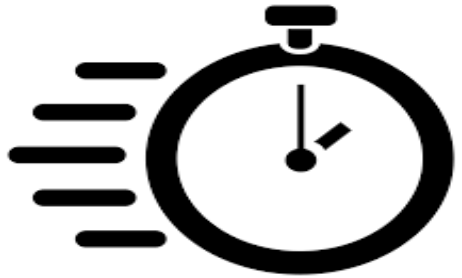
182	>	153
Precursor Ion	CID	Product Ion



w/ Argon Gas

The most complex aspect of adopting TQ methodology is the creation and implementation of MS/MS methods

Auto SRM can reduce method development time up to 10-fold



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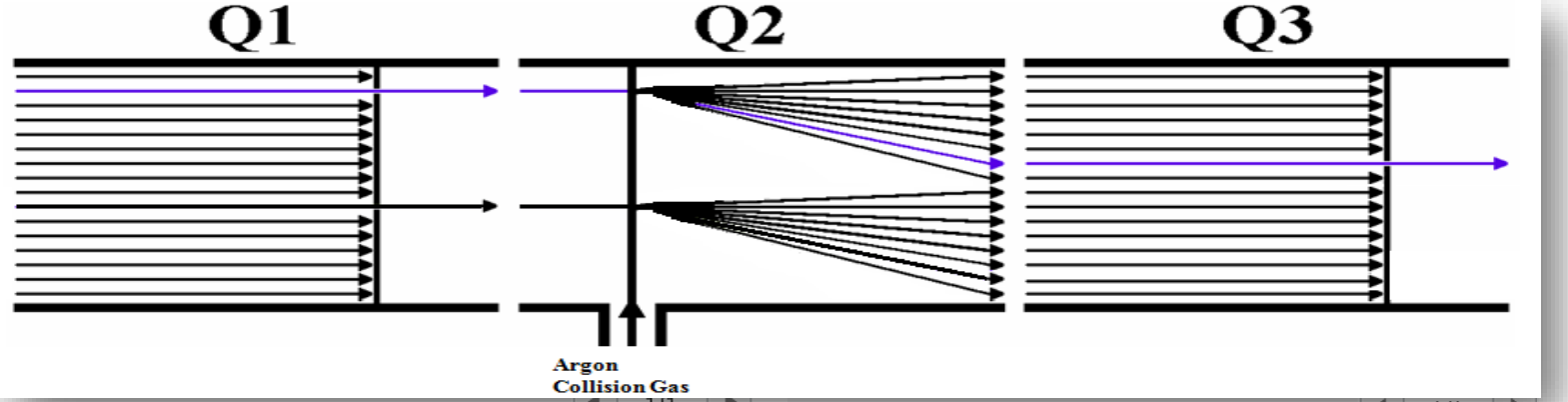
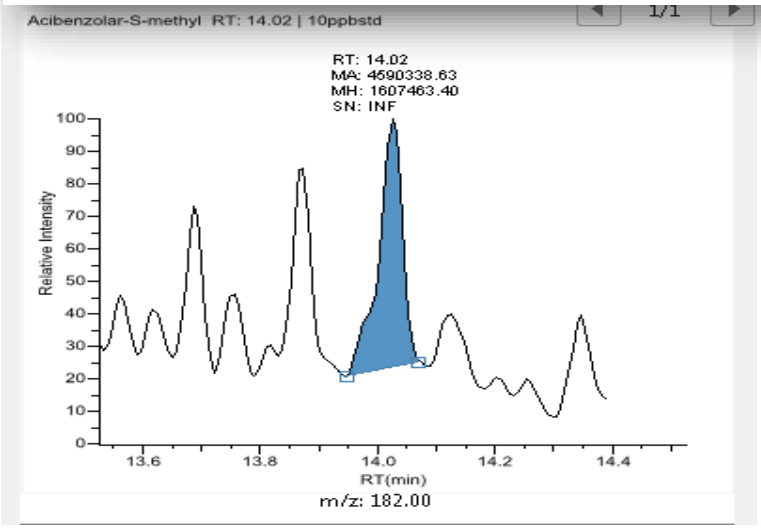
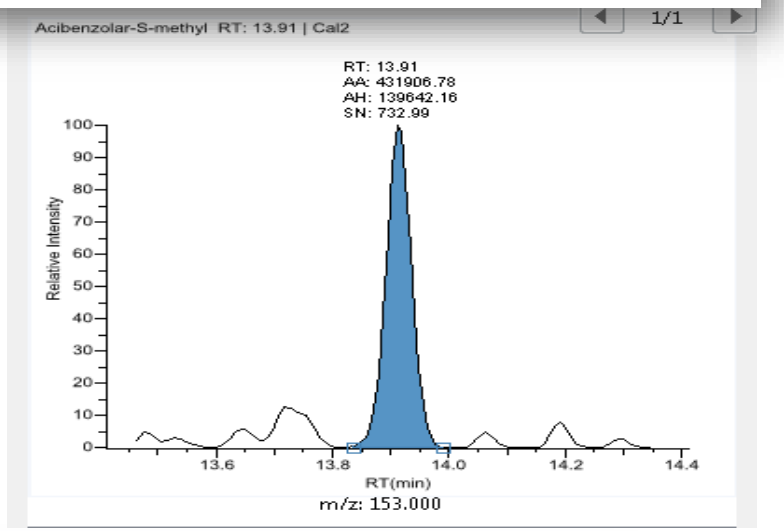
Triple Quad GC-MS: Selected Reaction Monitoring (SRM)





SIM on *m/z* 182



SRM on *m/z* 182 > 153

- Acibenzolar-S-Methyl in vegetable matrix

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The Benefits of Migration

- Enhanced selectivity
- Lower detection limits
- Better peak description
- Easier integration
- Faster, automated data processing
- Accurate results in heavy matrix
- Measure many compounds in one analytical run
- Maintain Regulatory Requirements

Auto SRM: Fast, Simple Route to Optimized SRM

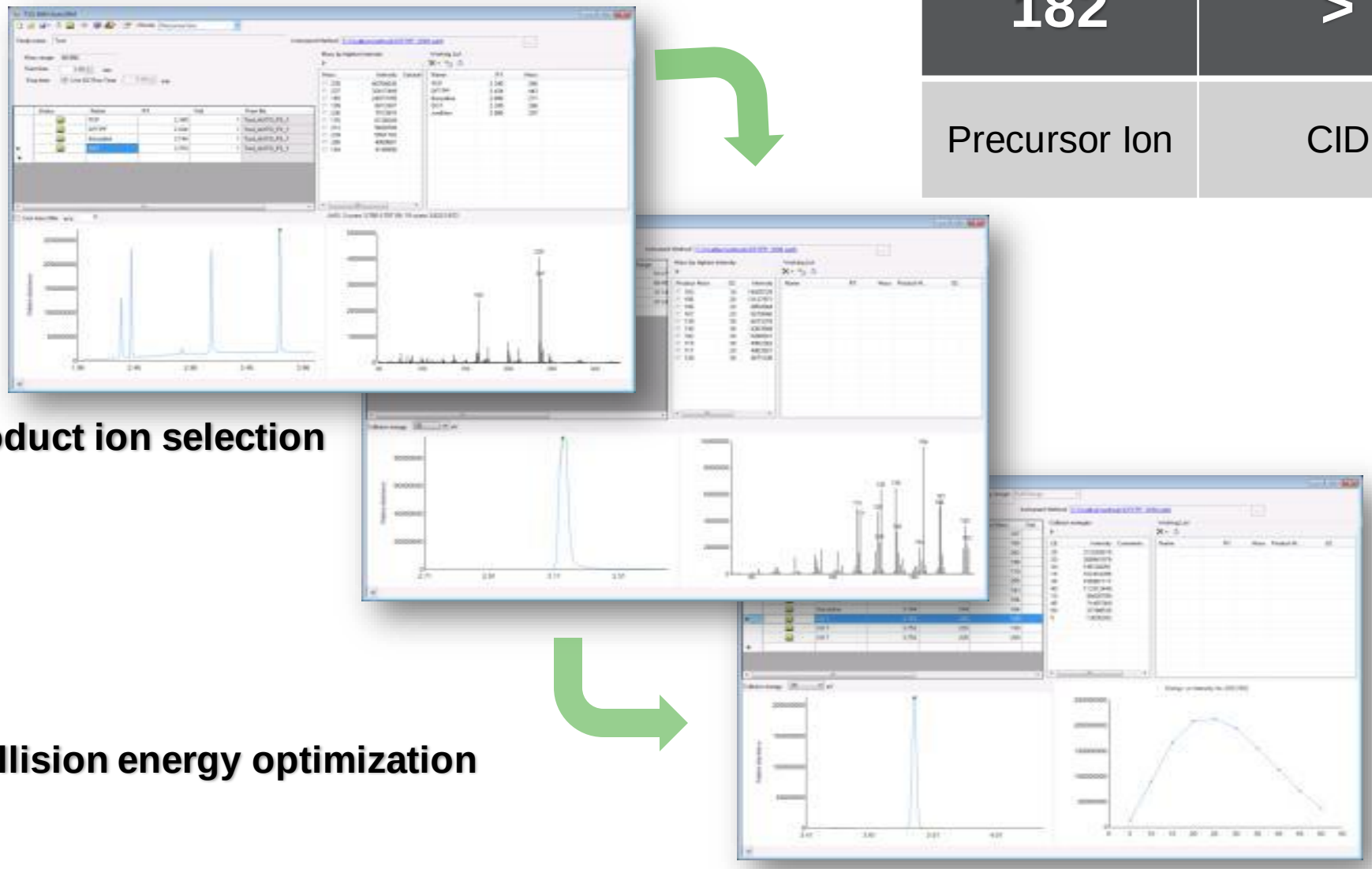
1

Precursor ion selection

182	>	153
Precursor Ion	CID	Product Ion

2

Product ion selection



3

Collision energy optimization

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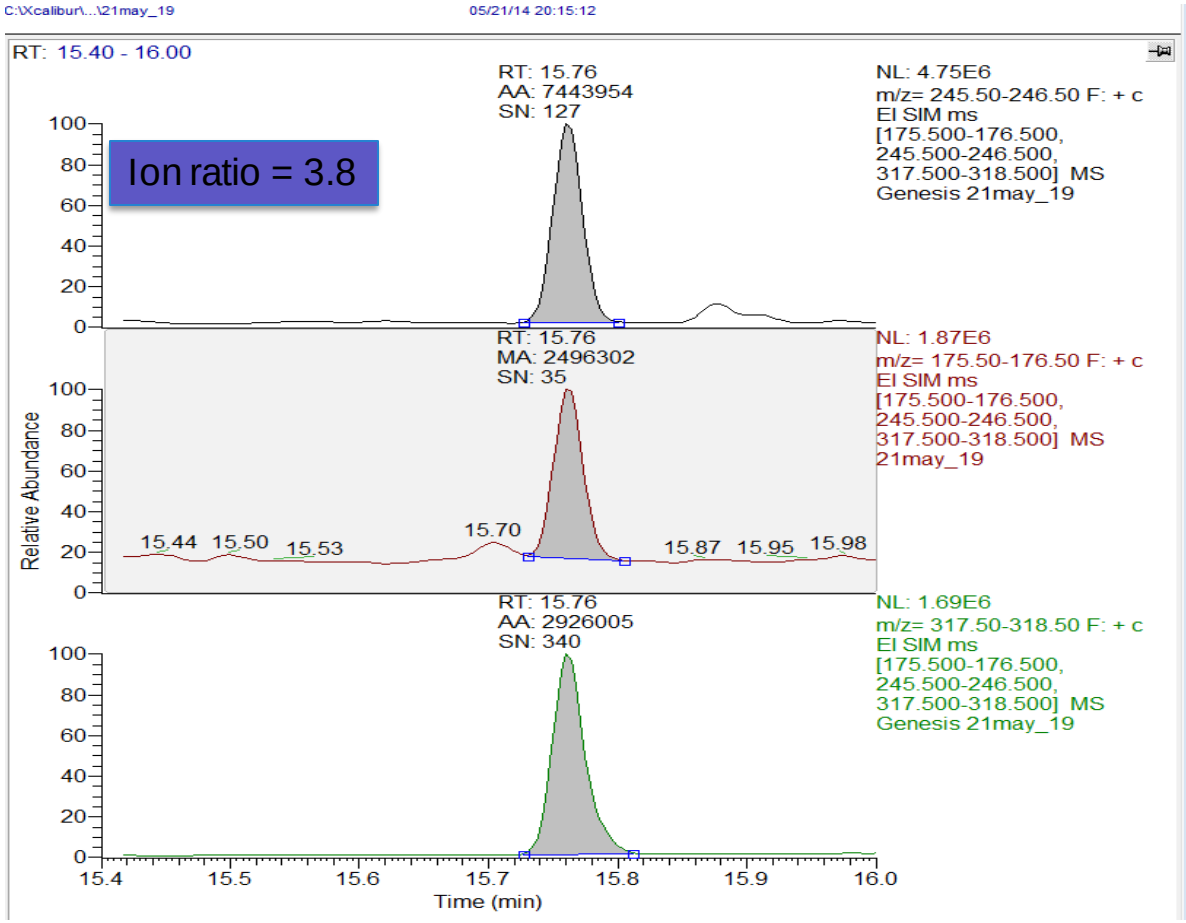
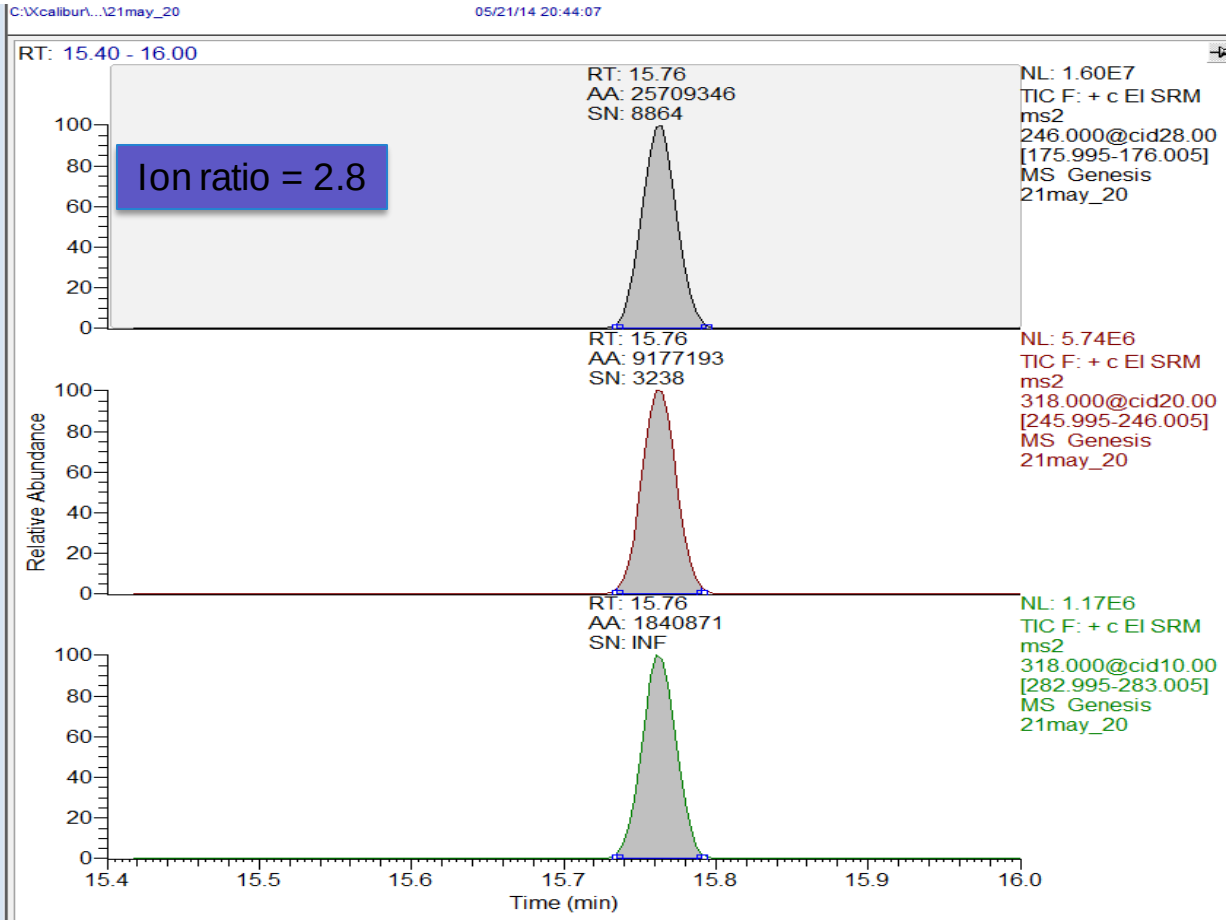
Selectivity: Selected Ion Monitoring (SIM) and SRM

DDE-p,p', **0.05** mg/kg in green tea, 1.0 uL splitless injection

SIM



SRM



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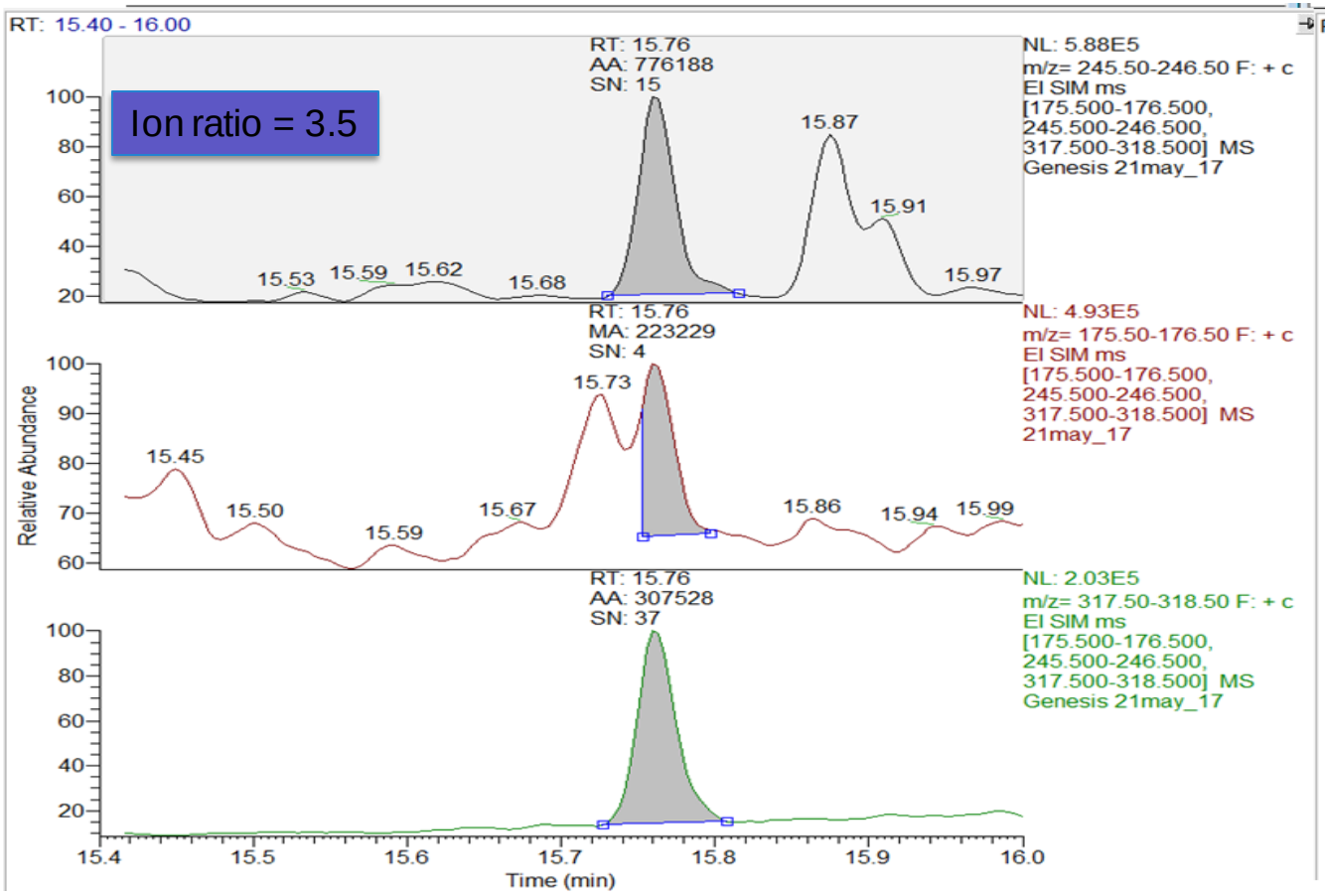
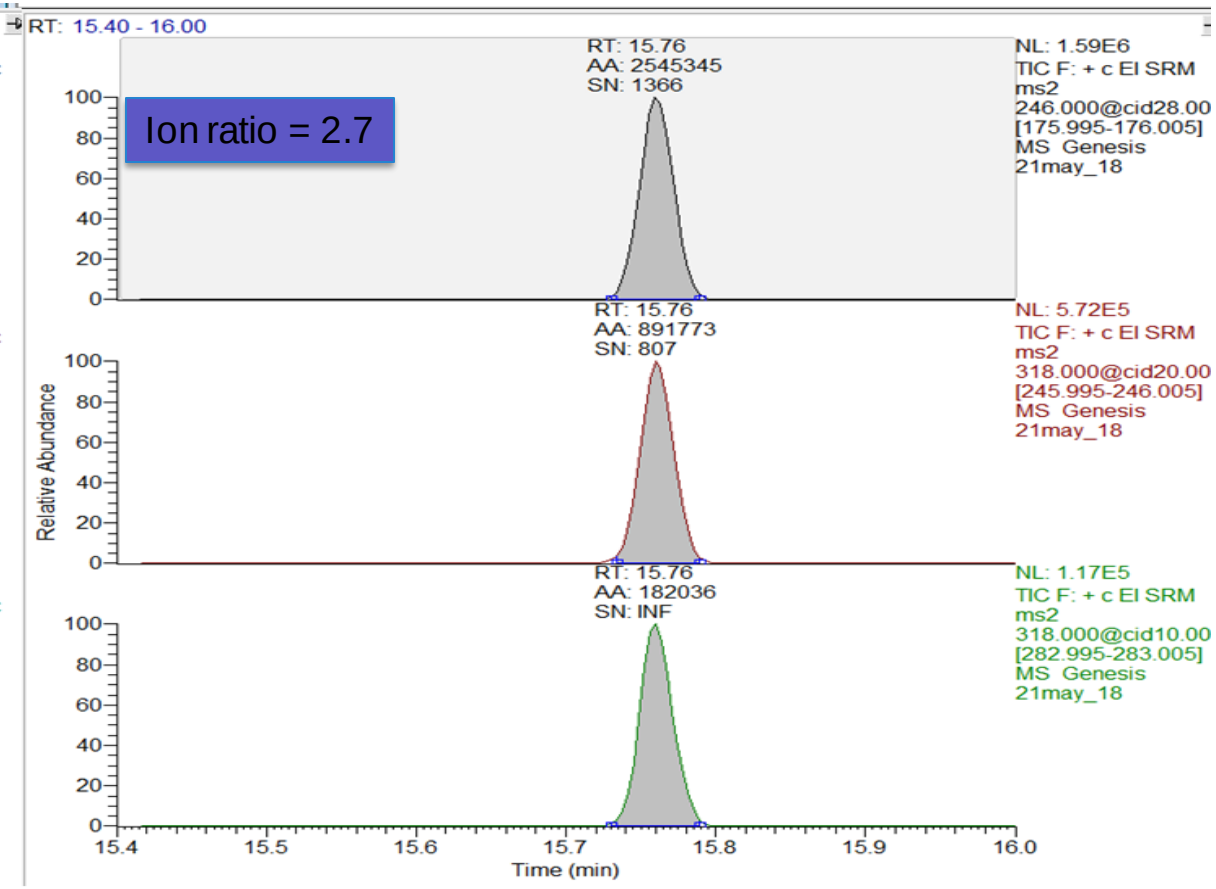
Selectivity: SIM and SRM

DDE-p,p', **0.005** mg/kg in green tea, 1.0 uL splitless injection

SIM



SRM



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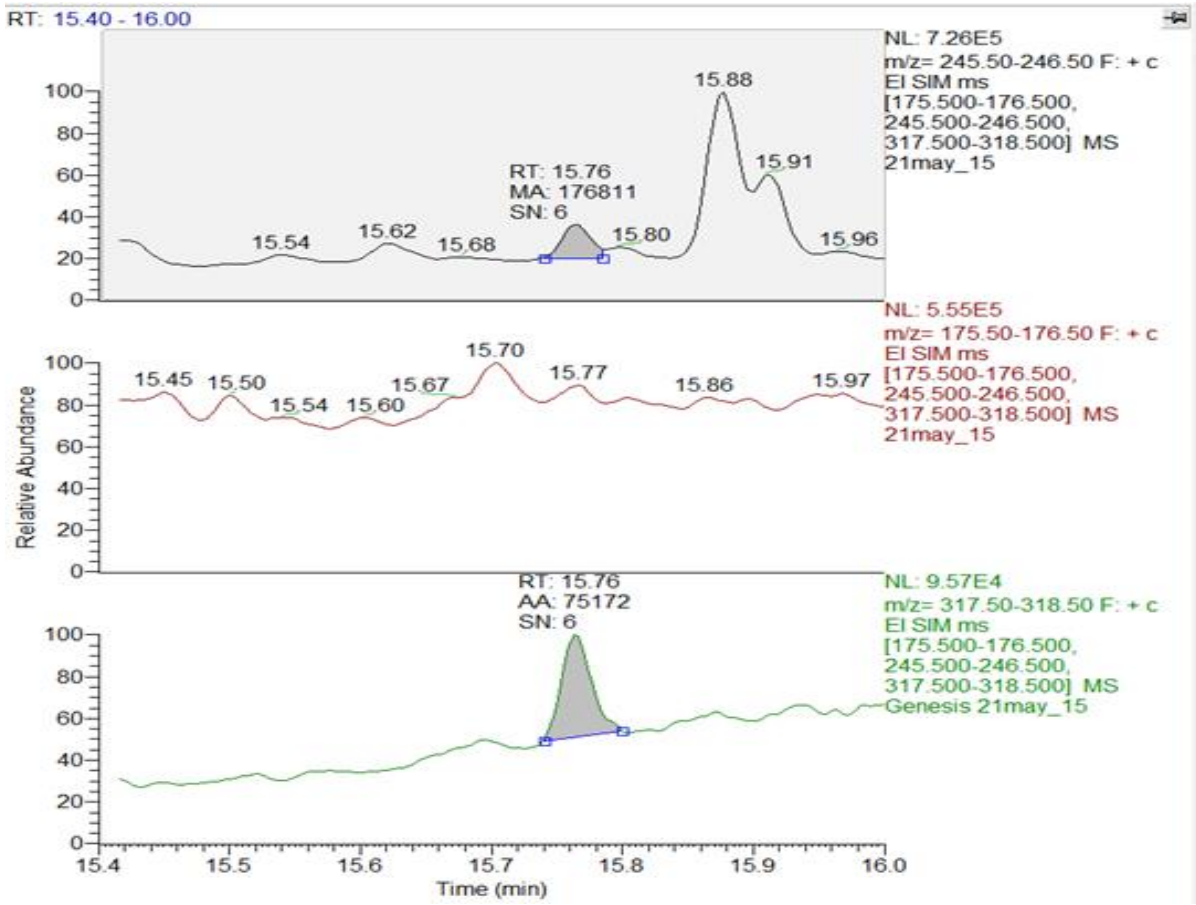
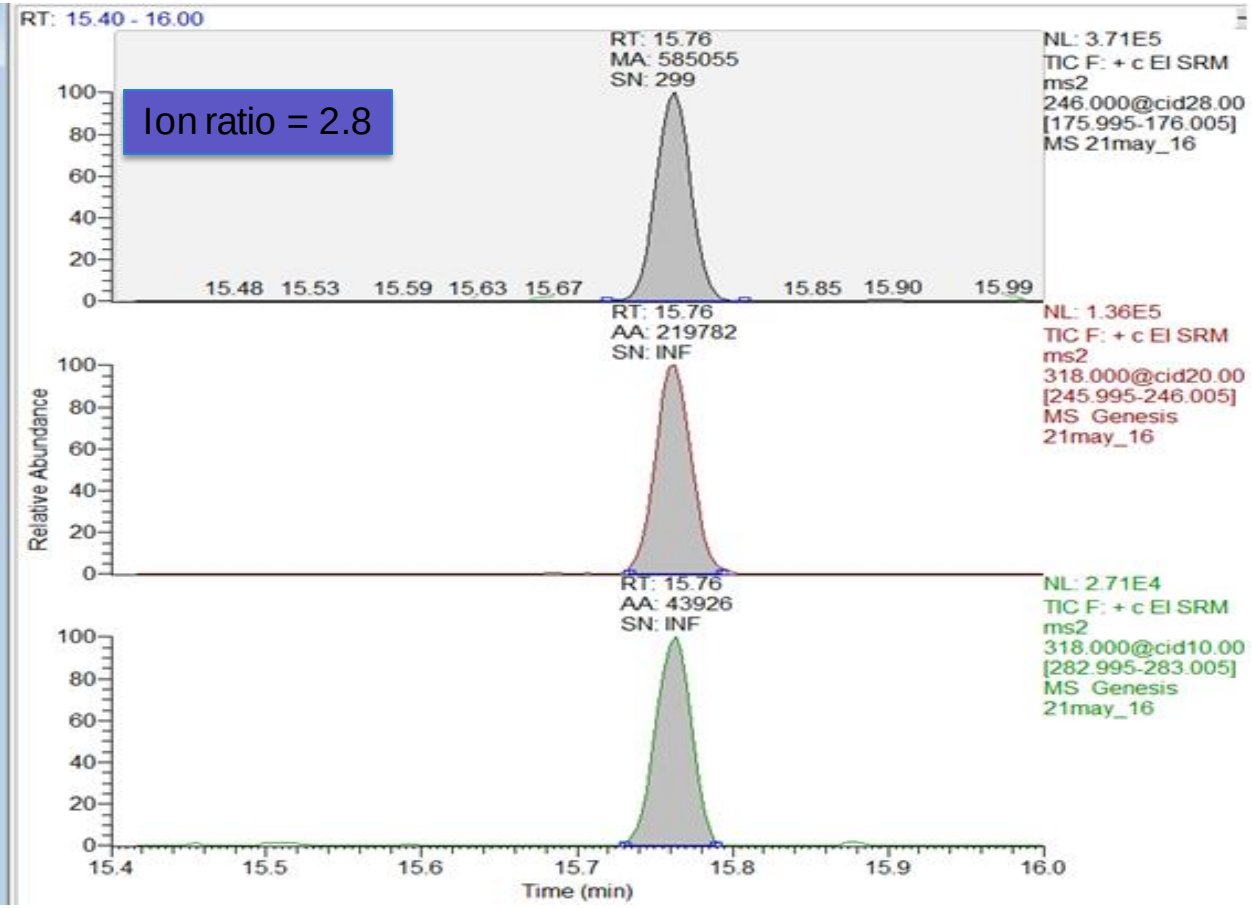
Selectivity: SIM and SRM

DDE-p,p', **0.001** mg/kg in green tea, 1.0 uL splitless injection

SIM



SRM



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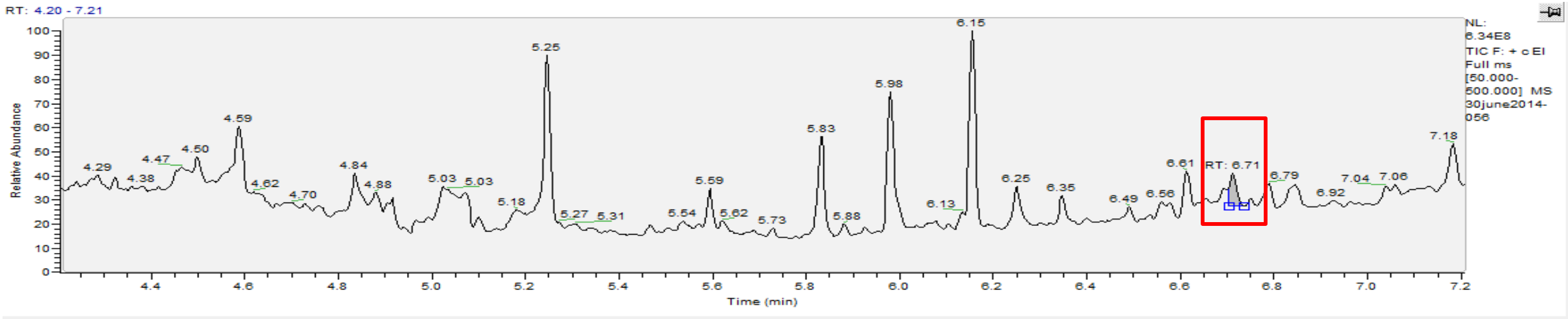
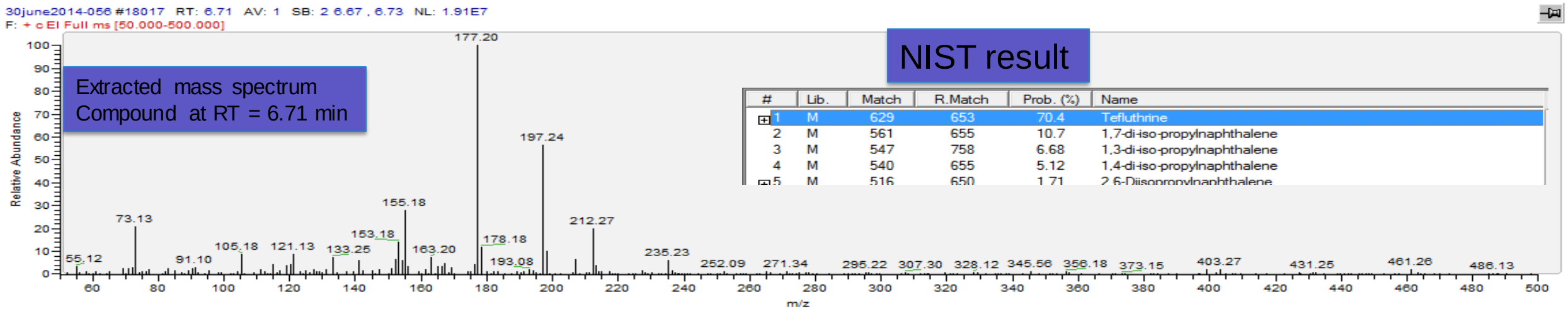
Simultaneous Full Scan and SRM Data Acquisition

Pesticides in baby food at 0.005 mg/kg.





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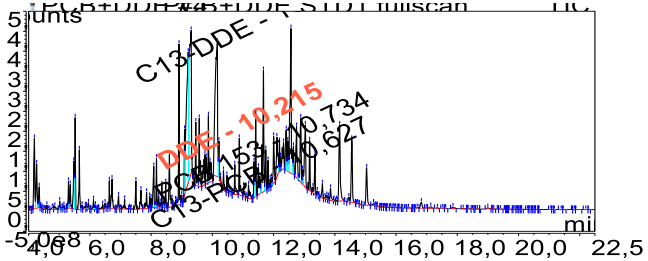
But What if the Chromatogram Looks Like This & I Don't Know What I'm Looking For?

- If you need to do both targeted AND untargeted screening at the same time fullscan data is required at the sensitivity needed for trace analysis



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Using Mass Spectrometers as Detectors in GC – Orbitraps

The Orbitrap GC-MS Family

Redefining Routine GC-MS

RP 60,000 (FWHM @ *m/z* 200)

EI/CI; Full-scan; Timed-SIM

Thermo Scientific™ Exactive™ GC system

Thermo Scientific™ Q Exactive™ GC system

Unprecedented Depth in Analysis

RP 120,000 (FWHM @ *m/z* 200)

EI/CI; Full-scan, Timed-SIM

MS/MS capability

The Technology Inside

Orbitrap mass analyzer

Incredible HRAM performance

Highly regarded Q Exactive GC system platform

Thermo Scientific™ TRACE™ 1310 GC System

Unique modular injector and detector design

Rapid heat cycling

Thermo Scientific™ ExtractaBrite™ Ion Source technology

Routine grade robustness

Patented RF lens

Removable without breaking vacuum

Portfolio positioning by application/workflow

Exactive GC

- Pesticide & contaminant screening & quan
- Environmental contaminants screening & quan
- Cosmetic s- Allergens
- Antidoping and forensic tox screening

Q Exactive GC

- Authenticy; food profiling,; extractable and leachables
- Emerging contaminants research
- Industrial research; product and materials characterization; petroleomics
- Targeted and untargeted metabolomics
- Pharmaceutical Impurity analysis; extractables and leachables

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Breakthrough in GC-MS Capability

The Power of Q Exactive GC

Resolution

Up to 120,000 at m/z 200

- Highest available
- Maximum selectivity
- Fast enough for GC!

Mass Accuracy

< 1ppm

- Every scan
- All concentrations
- In complex matrix
- Across the mass range
- Everyday!

Sensitivity

ppt

- In full scan
- High selectivity
- High spectral fidelity

Dynamic Range

>6 orders

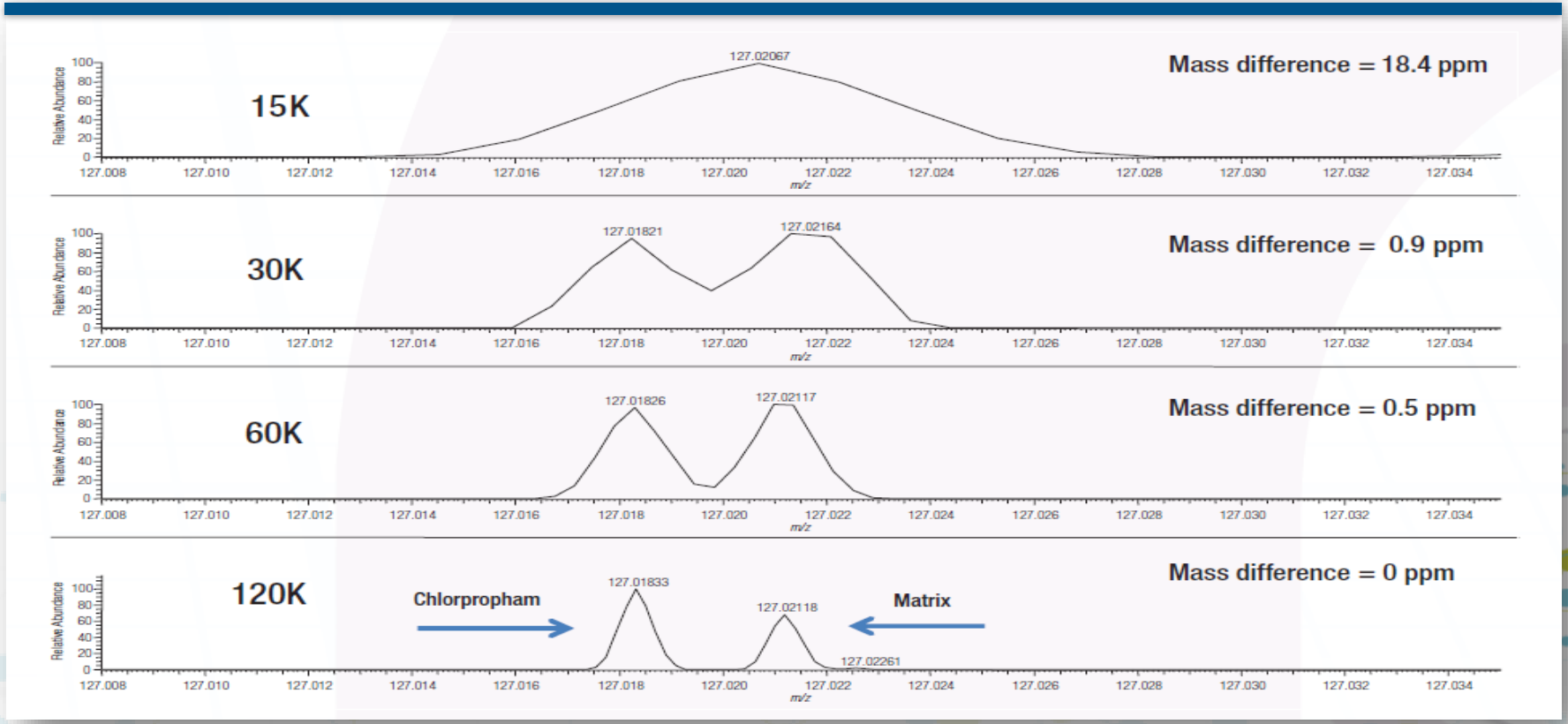
- Excellent coverage in sample profiling
- "Triple quad grade" quantitation in full scan

Breakthrough in GC-MS Performance

Highest selectivity and confidence with high resolving power

Chlorprophram

- 10 ng/g QuEChERS extract of leek
- Full scan with resolving power of >30k (FWHM @ m/z 200) provides interference free detection
- Excellent mass accuracy for confident identification



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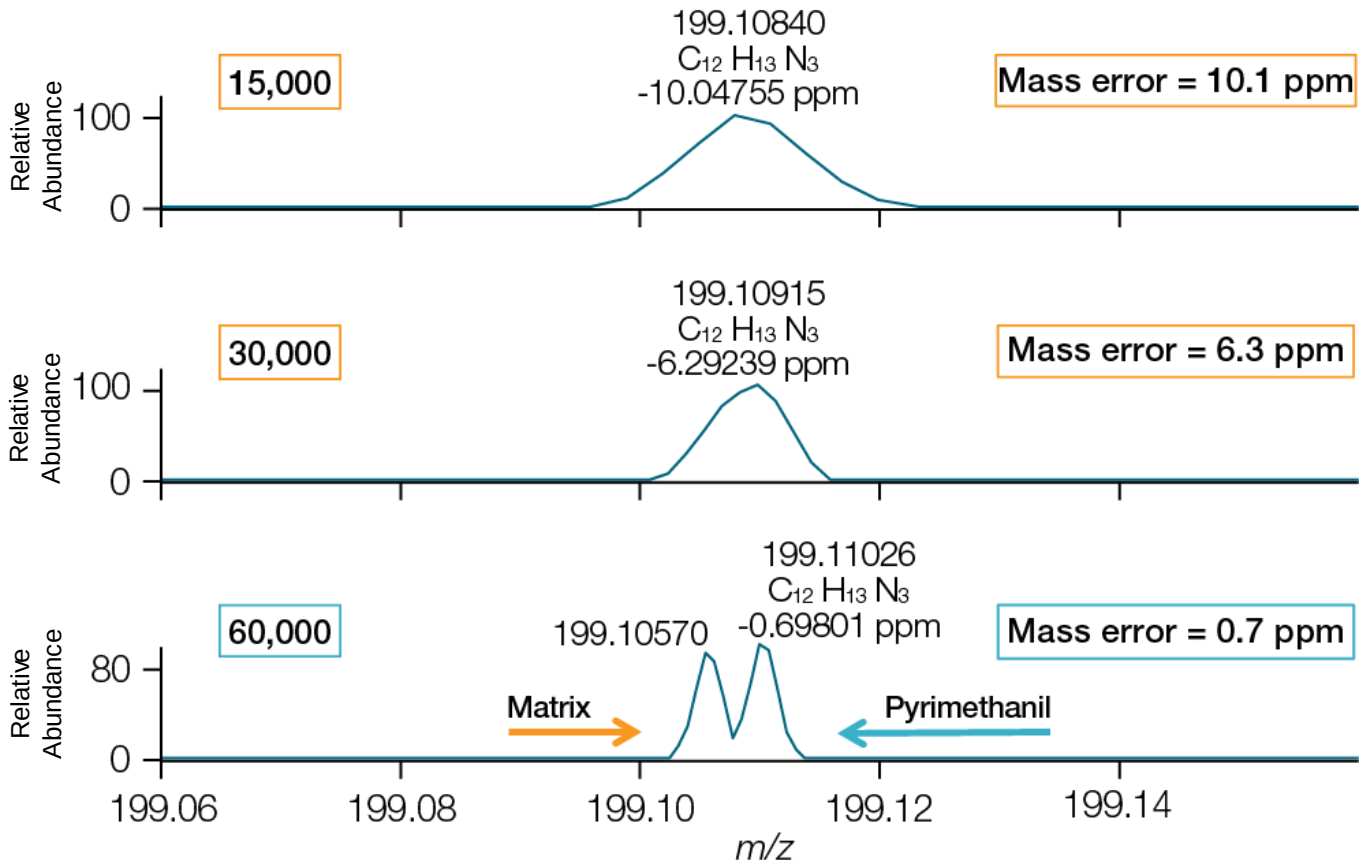
Resolving Power: Selectivity

Pyrimethanil in leek at 10 µg/Kg

< 5 ppm ID criteria



False negative

False negative

Positive Detection

High Selectivity ∴ high sensitivity *and* confidence in identification

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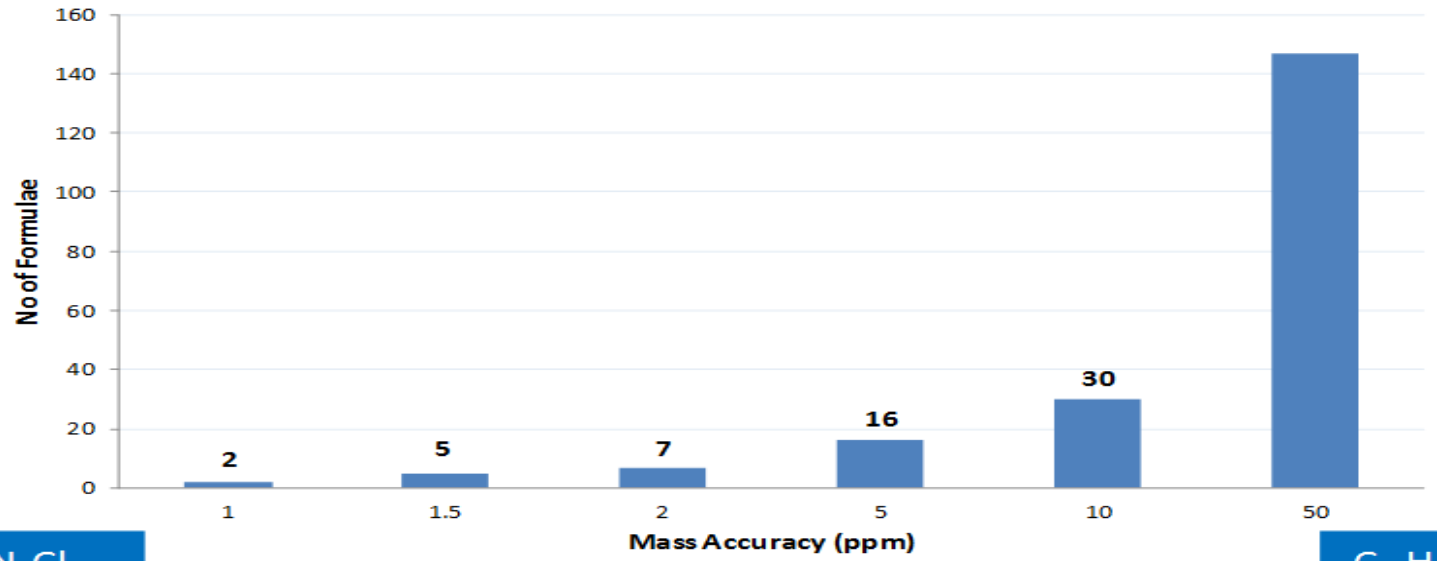
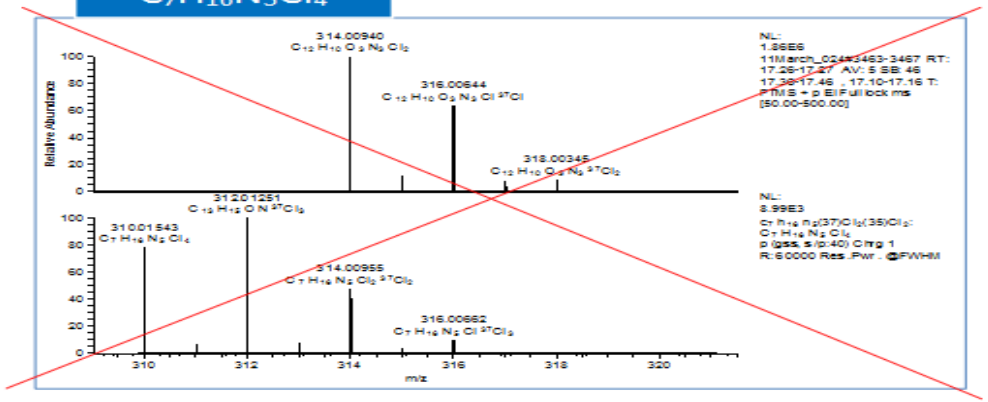
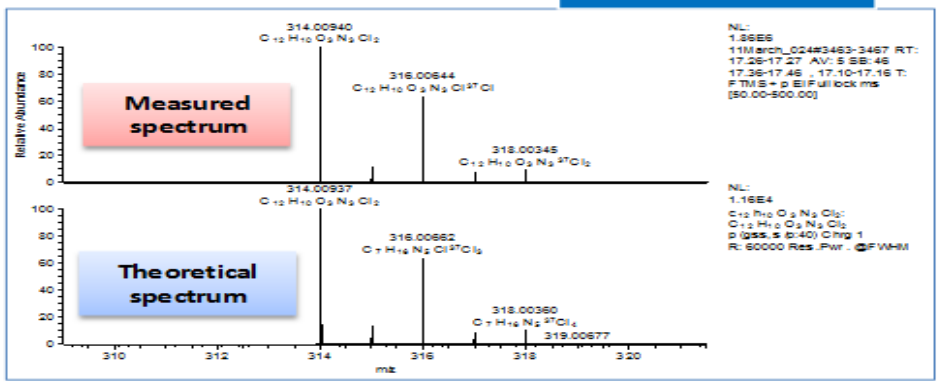
Compound ID Confirmation



$C_7H_{16}N_5Cl_4$



$C_{12}H_{10}N_5O_3Cl_2$



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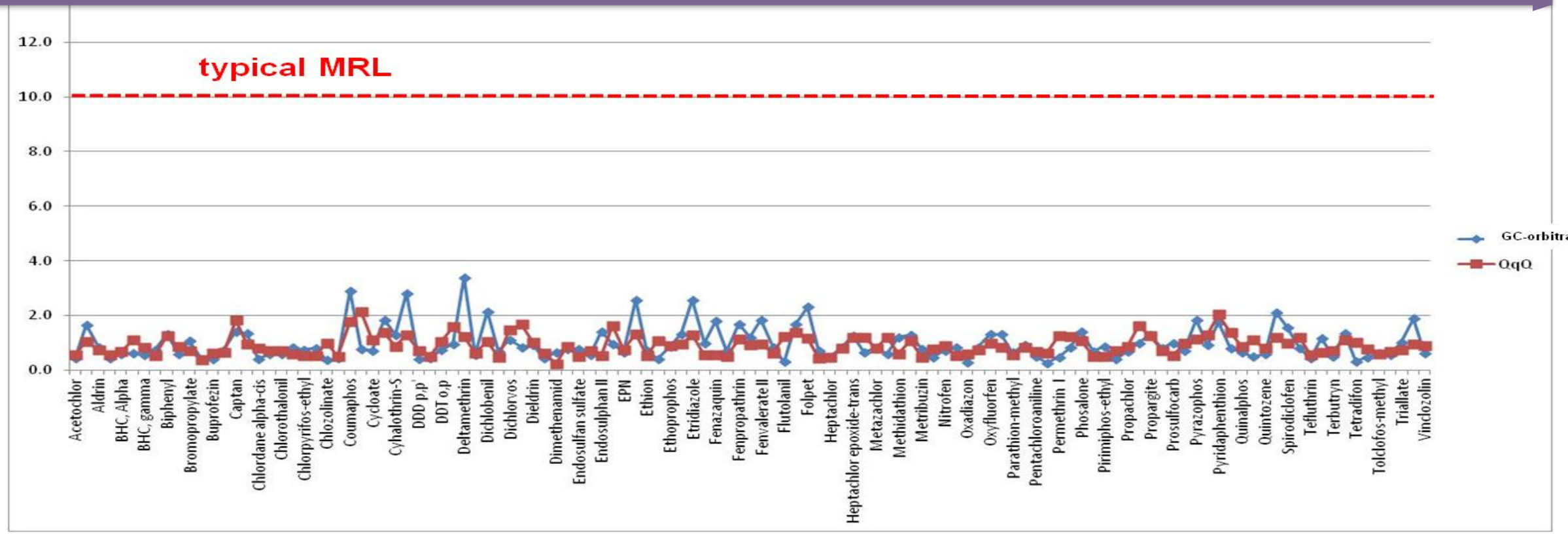
QQQ SRM vs Thermo Scientific Q Exactive Full Scan

Comparison QQQ in SRM and Q Exactive in Full Scan



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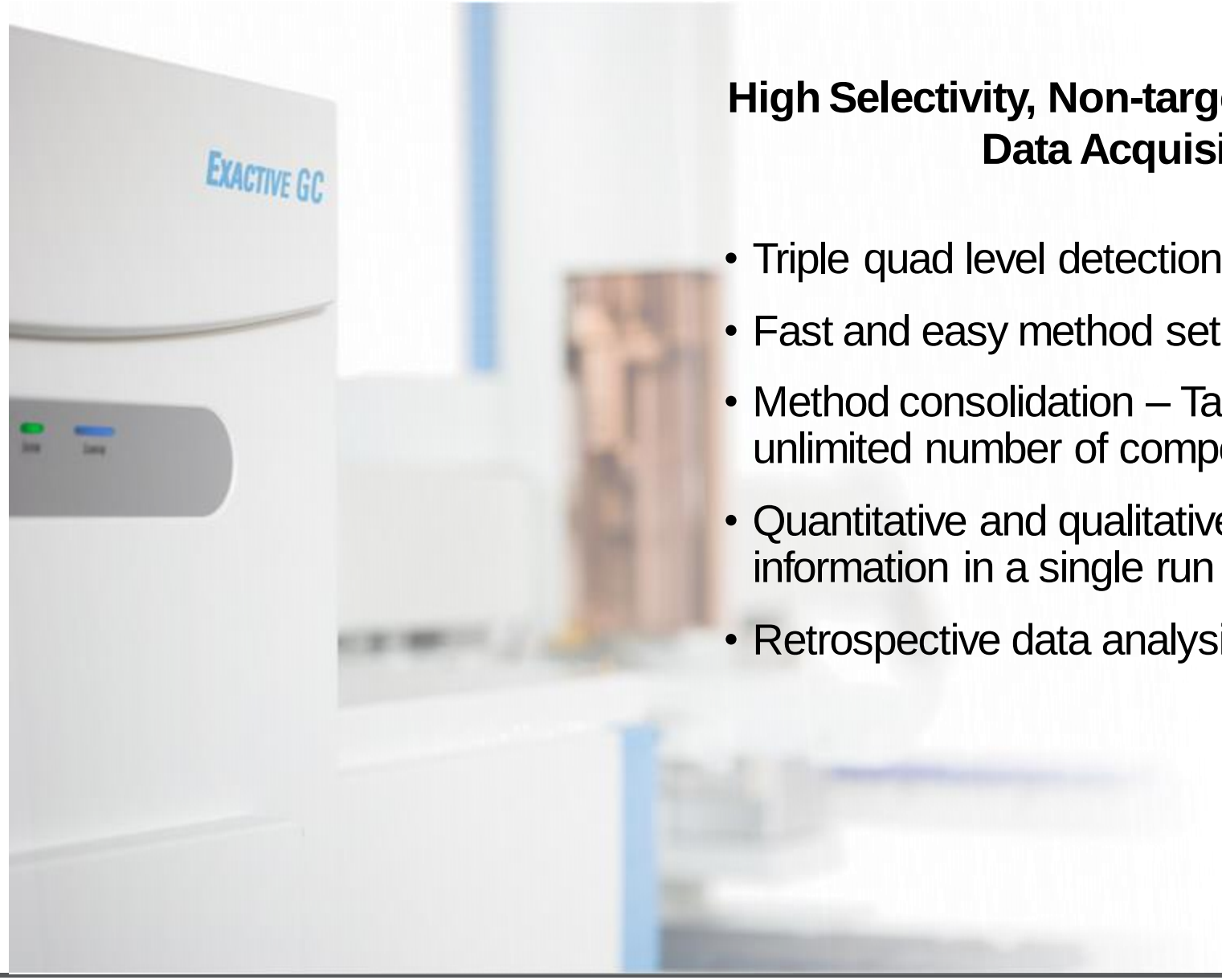
The Frontier of Routine GC-MS



High Selectivity, Non-targeted Data Acquisition

- Triple quad level detection limits
- Fast and easy method set-up
- Method consolidation – Target unlimited number of compounds
- Quantitative and qualitative information in a single run
- Retrospective data analysis

Join the Fun! *Cache a Chromeleon* Game

- Use your mobile device to complete challenges and earn a Charlie Chromeleon plush toy!
- If you are playing, you have earned points for attending this seminar. Be sure to scan the barcode on the desk outside the door.
- Ask booth staff for more details on how to play.

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Thank You

Please join me in the
Gas Chromatography
section of our booth where I'll
address additional comments and questions.